Determination of deformation-potential constants from quantum-limit cyclotron-resonance linewidths for Ge with anisotropic scattering

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Utilizing state-independent projection operators, we obtain a Lorentzian form of cyclotron-transition absorption spectra in the quantum limit. The linewidth formula is applied to determine the dilation and uniaxial deformation-potential constants (Ξ_d, Ξ_u) for anisotropic materials. By fitting the theoretical values to the experimental data, we obtain $\Xi_u = 18.0 \pm 0.6$ eV and $\Xi_d = -12.2 \pm 0.68$ eV for Ge.

For the conduction bands of Ge and Si, the constant energy surfaces are ellipsoidal, so that shear strains, as well as dilation strains, can produce the deformation potentials. From the symmetry property of Ge or Si, the deformation potentials can be described as just two independent potentials,[1] which are the dilation potential Ξ_d and the uniaxial shear potential Ξ_u.

Some research groups[2–5] for cyclotron resonance (CR) described the theoretical expression of cyclotron-resonance linewidth (CRLW) in terms of Herring-Vogt's equation[1] and determined the deformation potentials of Ge and Si by fitting the formula to their experimental data. However, this method is applicable for a limited case, since Herring-Vogt's equation is formulated in the classical limit ($k_B T \gg \hbar\omega$), where T is the temperature and ω the frequency of the eletromagnetic wave. On the other hand, most of CR theories[6–11] have the difficulty that the formulas are not applicable to the anisotropic scattering in the quantum limit ($k_B T \ll \hbar\omega$). Therefore, in this paper, we shall introduce a formula for the quantum-limit CRLW, using a projection operator technique.

At low temperatures, the transport phenomena of electrons in pure Ge is determined by the anisotropic scattering of acoustic phonons. When a static magnetic field ($\mathbf{B} = B\hat{z}$) is applied along the major axis of an ellipsoid, the Hamiltonian of the system is given by

$$H_{\rm tot} = \sum_{\alpha} \mathscr{E}_{N_\alpha, k_{z\alpha}} a_\alpha^\dagger a_\alpha + \sum_{\mathbf{q},s} \hbar\omega_{\mathbf{q},s} b_{\mathbf{q},s}^\dagger b_{\mathbf{q},s} + \sum_{\mathbf{q},s} \sum_{\alpha,\mu} V_{\mathbf{q},s} \langle \alpha | \exp(i\mathbf{q}\cdot\mathbf{r}) | \mu \rangle a_\alpha^\dagger a_\mu (b_{\mathbf{q},s} + b_{-\mathbf{q},s}^\dagger), \tag{1}$$

where $a_\alpha^\dagger$ (a_α) is the creation (annihilation) operator for an electron in the Landau state $|\alpha\rangle \equiv |N_\alpha, k_{y\alpha}, k_{z\alpha}\rangle$, N_α the Landau level index, $\mathbf{k}_\alpha$ the electron wave vector, and $\mathscr{E}_{N_\alpha, k_{z\alpha}}$ the Landau energy given by

$$\mathscr{E}_{N_\alpha, k_{z\alpha}} = (N_\alpha + 1/2)\hbar\omega_c + \hbar^2 k_{z\alpha}^2 / 2m_l + \mathscr{E}_C. \tag{2}$$

Here $\omega_c (\equiv eB/m_t)$ is the CR frequency of electrons, m_l (m_t) the longitudinal (transverse) effective mass of the electron, and $\mathscr{E}_C$ the bottom of the conduction band. In Eq. (1), $b_{\pm\mathbf{q},s}^\dagger$ ($b_{\pm\mathbf{q},s}$) is the creation (annihilation) operator for phonon in the state $|\pm\mathbf{q},s\rangle$, $\hbar\omega_{\mathbf{q},s}$ the phonon energy, $\mathbf{q}$ the phonon wave vector, s the index of phonon mode, and $V_{\mathbf{q},s}$ the coupling coefficient for the electron-phonon interaction.

In anisotropic solids such as Ge and Si, the sound speed $v_{\mathbf{q},s}$ of acoustic phonon is different for different direction of propagation. However, the difference is not so large,[12] and thus we assume that the sound speed is independent of the direction of propagation. Then we can define the coupling coefficient in Eq. (1) for longitudinal mode as

$$V_{\mathbf{q},L} = i(\hbar q / 2\rho_m \bar{v}_L)^{1/2} (\Xi_d + \Xi_u \cos^2\theta_{\mathbf{q}}) \tag{3}$$

and for the sum of two branches of transverse mode as

$$V_{\mathbf{q},T} = i(\hbar q / 2\rho_m \bar{v}_T)^{1/2} \Xi_u \sin\theta_{\mathbf{q}} \cos\theta_{\mathbf{q}}, \tag{4}$$

where $\theta_{\mathbf{q}}$ is the inner angle between the major ellipsoidal axis and $\mathbf{q}$, ρ_m is the mass density of the bulk, $\bar{v}_{L(T)} = (c_{L(T)}/\rho_m)^{1/2}$ is the average of the sound speed $v_{\mathbf{q},s}$ for each mode, $c_L = (3c_{11} + 2c_{12} + 4c_{44})/5$ and $c_T = (c_{11} - c_{12} + 3c_{44})/5$ are the elastic stiffness constants,[13] and $L(T)$ denotes the longitudinal (transverse) mode of the phonon.

Most of the CR theories[6–11] adopted state-dependent projection operators to obtain the CRLW functions from the Kubo formula. However, their functions failed to produce the two deformation potentials. In order to obtain the CRLW of Ge or Si, they made an approximation of isotropic electron-phonon scattering.[8,10,14,15] To overcome this problem, we introduce (state-independent) projection operators given by

$$PX \equiv \frac{\langle [X, J^-] \rangle}{\langle [J^+, J^-] \rangle} J^+, \quad P' \equiv 1 - P, \tag{5}$$

where $\langle\ \rangle$ denotes the grand canonical ensemble average and $J^\pm \equiv J_x \pm i J_y$ are the circular current operators of electrons. We shall use these projection operators of Eq. (5) and then obtain the formula for the CRLW by the same procedure as that of Ref. 11.

When a circularly polarized microwave with frequency ω and the electric-field amplitude E_0 is incident upon the system along the z axis, the absorption power density is given by

$$\mathscr{P}(\omega,\omega_c,T) = \left(\frac{E_0^2}{2\hbar\omega}\right) \times \frac{\langle[J^-,J^+]\rangle \mathrm{Re}[\Pi(\omega,\omega_c,T)]}{\{\omega-\omega_c-\mathrm{Im}[\Pi(\omega,\omega_c,T)]\}^2+\{\mathrm{Re}[\Pi(\omega,\omega_c,T)]\}^2}. \tag{6}$$

Here, $\Pi(\omega,\omega_c,T)$ is the averaged line-shape function given by

$$\Pi(\omega,\omega_c,T) = \frac{\Sigma_\alpha(N_\alpha+1)[f(\mathscr{E}_{N_\alpha+1,k_{z\alpha}})-f(\mathscr{E}_{N_\alpha,k_{z\alpha}})]\Gamma_\alpha(\omega,\omega_c,T)}{\Sigma_\alpha(N_\alpha+1)[f(\mathscr{E}_{N_\alpha+1,k_{z\alpha}})-f(\mathscr{E}_{N_\alpha,k_{z\alpha}})]}, \tag{7}$$

where $\Gamma_\alpha(\omega,\omega_c,T)$ is the energy-dependent line-shape function, which is the same as that given by Eq. (3.19) in Ref. 11 and $f(\mathscr{E}_{N_\alpha,k_{z\alpha}})$ the Fermi-Dirac distribution. In Eq. (6), $\mathrm{Im}[\Pi(\omega,\omega_c,T)]$ and $\mathrm{Re}[\Pi(\omega,\omega_c,T)]$ are related to the peak shift and linewidth of the CR absorption, respectively. Note that averaging over the electron distribution appears separately in the numerator and in the denominator in Eq. (7). Therefore, the averaged line-shape function may be more manageable than the other formulas.[6–11]

We shall make some approximations under the condition of the quantum limit. First, the peak shift of $\mathrm{Im}[\Pi(\omega,\omega_c,T)]$ is ignored in comparison with ω_c. Second, the Fermi-Dirac distribution is approximated by the Maxwell-Boltzmann distribution or ignored in comparison with the phonon distribution function. Third, we take into account only the transitions from the lowest Landau level ($N_\alpha=0$) to excited states, since most of electrons reside on the lowest Landau level. Fourth, we replace $\mathrm{Re}[\Pi(\omega,\omega_c,T)]$ by $\mathrm{Re}[\Pi(\omega,\omega,T)]$, since $\mathrm{Re}[\Pi(\omega,\omega_c,T)]$ is very slowly varying function of ω_c near the resonance region. In this case, the absorption power density of Eq. (6) can be rewritten as

$$\mathscr{P}(\omega,\omega_c,T) \simeq \mathscr{P}_{\max}(\omega,T)\frac{\xi(\omega,T)^2}{(\omega-\omega_c)^2+\xi(\omega,T)^2}, \tag{8}$$

where the maximum absorption power intensity is

$$\mathscr{P}_{\max}(\omega,T) = (eE_0)^2 n(\omega,T)/m_t\xi(\omega,T) \tag{9}$$

and the averaged relaxation rate is defined as

$$\xi(\omega,T) \equiv \mathrm{Re}[\Pi(\omega,\omega,T)] \simeq \frac{\hbar}{\sqrt{2\pi m_l k_B T}}\int_{-\infty}^{\infty} dk_z \exp(-\hbar^2 k_z^2/2m_l k_B T) \times \gamma(\omega,T,k_z), \tag{10}$$

which has a form of the Boltzmann average of the energy-dependent relaxation rate $\gamma(\omega,T,k_z)$, defined as the real part of the energy-dependent line-shape function. In Eq. (9), the electron concentration $n(\omega,T)$ is given by

$$n(\omega,T) = g_v\omega(m_l m_t^2 k_B T/8\pi^3\hbar^4)^{1/2} \times \exp[-(\mathscr{E}_C-\zeta)/k_B T]/\sinh(\hbar\omega/2k_B T), \tag{11}$$

where ζ is the chemical potential for an electron and the weight parameter g_v shall be discussed later. Note that the averaged relaxation rate is equal to the half CRLW, since the spectrum of the absorption power intensity for ω_c has a form of Lorentzian shape. In Eq. (10), the energy-dependent relaxation rate is given by

$$\gamma(\omega,T,k_z) = \gamma_L^{(+)}+\gamma_L^{(-)}+\gamma_T^{(+)}+\gamma_T^{(-)} \tag{12}$$

where the subscript "$L(T)$" and the superscript "$+(-)$," respectively, represent the longitudinal (transverse) mode of phonon and the phonon absorption (emission) process. Each part of Eq. (12) is given by

$$\gamma_L^{(\pm)} = \left(\frac{g_v\Xi_u^2}{4\pi\hbar\bar{v}_L^2\rho_m}\right)\sum_{N=0,1}\int_{a_1^\pm}^{a_2^\pm} dq_z (q_L^{\pm 2}+q_z^2) \times\left(D+\frac{q_z^2}{q_L^{\pm 2}+q_z^2}\right)^2 \times K(0,N;\hbar q_L^{\pm 2}/2m_t\omega_c)\left[\begin{pmatrix}0\\1\end{pmatrix}+N\left(\hbar\bar{v}_L\sqrt{q_L^{\pm 2}+q_z^2}\right)\right] \tag{13}$$

and

$$\gamma_T^{(\pm)} = \left(\frac{g_v\Xi_u^2}{4\pi\hbar\bar{v}_T^2\rho_m}\right)\sum_{N=0,1} \times\int_{a_3^\pm}^{a_4^\pm} dq_z \frac{q_T^{\pm 2}q_z^2}{q_T^{\pm 2}+q_z^2}K(0,N;\hbar q_T^{\pm 2}/2m_t\omega_c) \times\left[\begin{pmatrix}0\\1\end{pmatrix}+N\left(\hbar\bar{v}_T\sqrt{q_T^{\pm 2}+q_z^2}\right)\right], \tag{14}$$

where the limits ($a_i^\pm$) of the integrations in Eqs. (13) and (14) are determined from the energy-momentum conservation for each process, $K(0,N;t)=(t-N)t^N\exp(-t)/N!$, $N(\hbar\omega_{\mathbf{q},s})$ Bose-Einstein distribution for phonon with an energy of $\hbar\omega_{\mathbf{q},s}$, $D\equiv\Xi_d/\Xi_u$, and $q_{L(T)}^\pm=\{[(1-N)\hbar\omega-\hbar^2(q_z^2\pm 2k_z q_z)/2m_l]^2/(\hbar\bar{v}_{L(T)})^2-q_z^2\}^{1/2}$.

In Eqs. (11), (13), and (14), g_v is inserted, since one of peaks in a CR absorption spectrum is constructed by the electrons in the valleys with the same inner angle between the major axes of the valleys and the direction of the magnetic field **B**. The number of CR peaks is different according to the direction of **B**. In the case of a peak produced by the electrons in the valley with the major axis parallel to **B**, the cyclotron frequency is $\omega_c=eB/m_t$ and $g_v=1$ for Ge. For a peak related to the major axis perpendicular to **B**, $\omega_c=eB/(m_t m_l)^{1/2}$ and $g_v=1$ for Ge. For Si, the values of g_v are different for the different directions of **B**.

We shall determine the values of Ξ_u and Ξ_d from fitting the derived half CRLW of Eq. (10) to suitable experimental data. One of the candidates may be the anisotropy ratio about

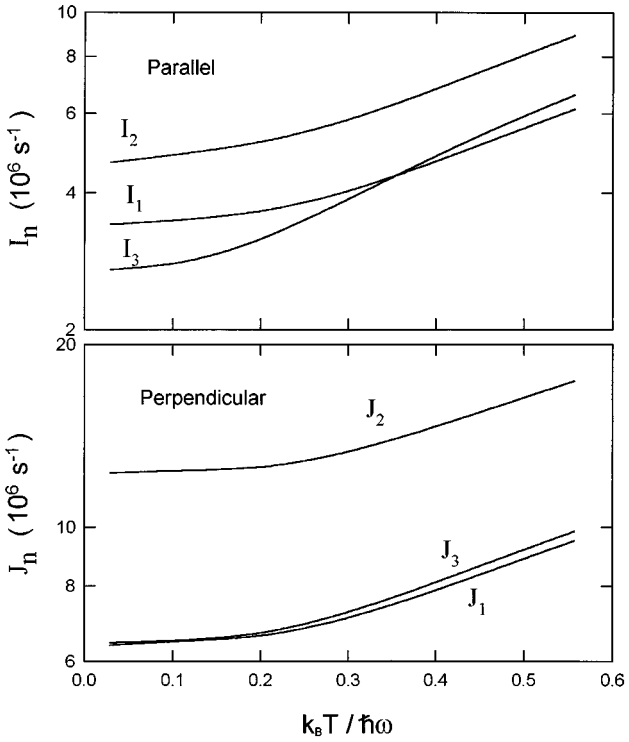

FIG. 1. Integrals I_n and J_n as functions of temperatures at $\omega = 446$ GHz for pure Ge.

the half CRLW. For a peak related to the major axis parallel to **B**, the half CRLW from Eq. (10) can be written as

$$\xi_{\parallel} = \Xi_u^2 (I_1 D^2 + I_2 D + I_3), \tag{15}$$

where I_n are the intergals for the coefficients of D. For a peak related to the major axis perpendicular to **B**, m_t and m_l are replaced by $(m_t m_l)^{1/2}$ and m_t, and $\sin\theta_{\mathbf{q}}$ and $\cos\theta_{\mathbf{q}}$ in Eqs. (3) and (4) by $\cos\theta_{\mathbf{q}}$ and $\sin\theta_{\mathbf{q}}$, respectively, since the coordinate system is rotated perpendicular to the former. Then we get the half CRLW as

$$\xi_{\perp} = \Xi_u^2 (J_1 D^2 + J_2 D + J_3), \tag{16}$$

where J_n also are the intergals for the coefficients of D. The anisotropy ratio of the half CRLW's is defined as

$$\frac{\xi_{\perp}}{\xi_{\parallel}} = \frac{J_1 D^2 + J_2 D + J_3}{I_1 D^2 + I_2 D + I_3}, \tag{17}$$

which is the function of D for a temperature and a resonance frequency.

Among the physical parameters for Ge, the elastic stiffness constants[16] are given by $c_{11} = 1.29 \times 10^{11}$ N/m^2, $c_{12} = 0.48 \times 10^{11}$ N/m^2, and $c_{44} = 0.67 \times 10^{11}$ N/m^2. The other values are given in Ref. 15. Then the values of I_n and J_n for $\omega = 446$ GHz are given in Fig. 1. Using these curves, the anisotropy ratio of Eq. (17) is plotted as functions of D, for some temperatures as shown in Fig. 2. The experimental data of Ito, Kawamura, and Fukai[3] show that the anisotropy ratio is almost constant for the range of 1.6 ~ 4.2 K and a wavelength of 6 mm, that is, in the classical limit. On the other hand, Murase, Enjouji, and Otsuka[5] argued that the

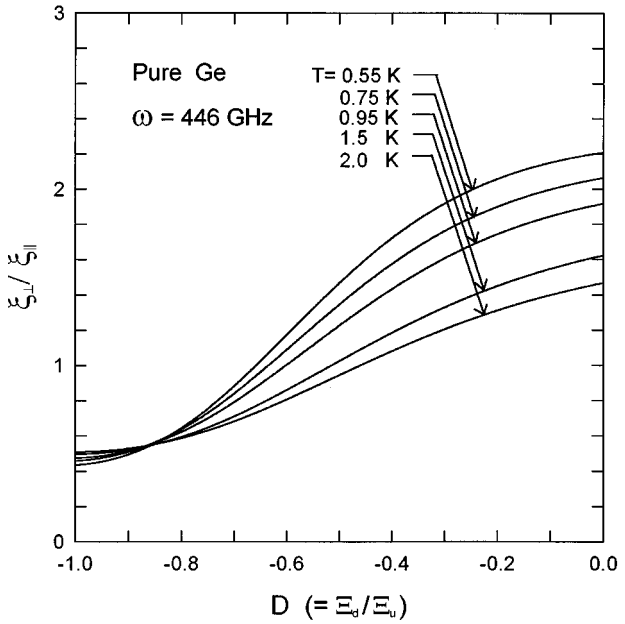

FIG. 2. Theoretical curves of the anisotropy ratio of the half CRLW's in pure Ge, as functions of D at $\omega = 446$ GHz.

anisotropy ratio decreases as the temperature increases for the range of 0.55 ~ 4.2 K with 446 GHz angular frequency, that is, in the quantum limit. Therefore, we get $D = -0.68 \pm 0.03$ from fitting the curves of Fig. 2 to the experimental data of Murase, Enjouji, and Otsuka.[5]

To get the value of the uniaxial deformation constant Ξ_u, we shall use a recent experimental data[14] related to the temperature dependence of CRLW for pure Ge in the quantum limit. When we put $\lambda = 220$ μm and take the direction of the applied magnetic field to be parallel to the $\langle 111 \rangle$ direction, we obtain $\Xi_u = 18.0 \pm 0.6$ eV from fitting the theoretical values calculated by using the given value of D to the experimental data. From these results, we obtain $\Xi_d = -12.2 \pm 0.68$ eV for Ge. The present result for the deformation potentials is similar to other results, as shown in Table I. In the quantum limit, the temperature dependence of half CRLW agrees well with the experimental data, as shown in Fig. 3, where the value of the half CRLW of the longitudinal mode relative to the transverse one is about 0.15–0.30 in the range of the quantum limit. At extremely low temperatures, the CRLW is independent of temperature as Meyer predicted.[24]

In summary, using the state-independent projection operators of Eq. (5), we presented the CRLW formula that is available to determine the two deformation potentials in the quantum limit. This formula was applied to Ge. For Ge, we obtained $D = -0.68 \pm 0.03$ from fitting the calculated anisotropy ratio of Eq. (17) to the experimental data[5] and $\Xi_u = 18.0 \pm 0.6$ eV from fitting the temperature dependence of the half CRLW obtained by using the given value of D to the other experimental data.[14] From these two values, we got $\Xi_d = -12.2 \pm 0.68$ eV. These results are similar to some other result as shown in Table I. In Fig. 3, the temperature dependence of CRLW in quantum limit is in better agreement with the experimental data than other results.[8,10,14,15] Also, we see that the contribution of transverse phonons to the CRLW is much larger than the longitudinal one in the

TABLE I. Deformation-potential constants from various experimental and theoretical methods for Ge.

Ξ_u (eV)	$D(=\Xi_d/\Xi_u)$	Ξ_d (eV)	Ref.
18.0 ± 0.6	-0.68 ± 0.03	-12.2 ± 0.68	Present work
20	-0.67	-13.5	2 [a]
18.7 ± 0.2	-0.561	-10.5 ± 0.5	3 [a]
19.3 ± 0.2	-0.636 ± 0.011	-12.3 ± 0.5	4 [a]
17.3			17 [b]
19.2 ± 0.4			18 [b]
16.0 ± 1.6			19 [c]
16.2 ± 0.4			20 [d]
18.0 ± 0.5			21 [e]
$15.4\sim19.5$			22 [f]
17.0 ± 0.2			23 [g]

[a]Cyclotron-resonance linewidth in the classical limit.
[b]Piezoresistance.
[c]Acoustoelectric effect.
[d]Influence of uniaxial stress on indirect absorption edge.
[e]Free-carrier piezobirefregence.
[f]Optical determination for donor impurities.
[g]Electronic effect in elastic constant C_{456}.

quantum limit and the CRLW is independent of temperature in the extremely low temperature region, as Meyer predicted.[24] Unfortunately, the deformation potentials of Si could not be determined, due to the lack of experimental information. If suitable experiments are available, Ξ_u and Ξ_d can be obtained for Si by the same technique.

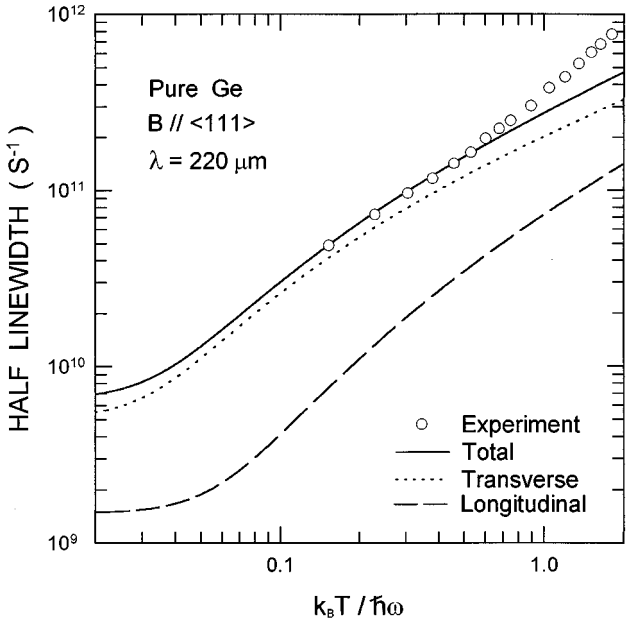

FIG. 3. Temperature dependence of the half CRLW in pure Ge at $\lambda=220$ μm and with the magnetic field along the $\langle 111\rangle$ direction. The dotted line and the broken line, respectively, show the half CRLW's, due to the transverse and the longitudinal mode of phonons. The solid line shows the total half CRLW. The open circles show the experimental data of Kobori, Ohyama, and Otsuka.

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